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Steric structure of phosphorus-containing heterocycles. Communication 37. 2-Phenoxy-5,6-benz-1-3,2-dioxaphosphepines with tetracoordinated phosphorus atom

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Abstract

1. 2-Phenoxy-2-oxo(thiono, seleno)-5,6-benz-1,3,2-dioxaphosphepines in solutions of nonpolar solvents are characterized by an equilibrium of two chair-like forms, which in the case of the sulfide and selenide is shifted in the direction of a conformer with an equatorial orientation of the phenoxyl group; in the oxide, at equilibrium, the proportions of two conformers are approximately the same. In solutions of polar solvents, a three component equilibrium is observed for the oxide, in which the flexible forms as well as the chair-like forms are present. 2. In accordance with the dipole moments and Kerr effect data, in all conformations, the compounds studied are characterized by a gauche conformation of the phenyl group in relation to the P=O (P=S, P=Se) bond and by an orthogonal disposition of the benzene ring π-orbitals and the p-unshared electron pair on the exocyclic oxygen atom. © 1986 Plenum Publishing Corporation.

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